

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX012720\
 Data File : VX014725.D
 Acq On : 27 Jan 2020 14:44
 Operator : JC/SP
 Sample : L1236-01
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMP-1

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.070	26	30	43	rBV	1310768	1564798	2.61%	1.359%
2	1.472	93	96	126	rBV	37435315	59887969	100.00%	52.011%
3	2.119	193	202	206	rBV	9675723	17431449	29.11%	15.139%
4	4.326	551	564	582	rBV	4894412	12958826	21.64%	11.254%
5	5.490	745	755	768	rBV	255300	740264	1.24%	0.643%
6	5.655	768	782	794	rVV	450171	1268766	2.12%	1.102%
7	6.057	838	848	856	rBV	282654	743311	1.24%	0.646%
8	6.849	969	978	991	rVB	710760	1661622	2.77%	1.443%
9	7.288	1039	1050	1069	rBV	3245595	6500606	10.85%	5.646%
10	8.709	1276	1283	1290	rBV	1532023	2321201	3.88%	2.016%
11	10.105	1507	1512	1521	rVB	1469472	2022087	3.38%	1.756%
12	10.361	1545	1554	1559	rBV	1425135	1967226	3.28%	1.708%
13	11.129	1675	1680	1685	rBV	1237749	1666514	2.78%	1.447%
14	12.074	1830	1835	1842	rVB	1559090	1949511	3.26%	1.693%
15	12.263	1861	1866	1878	rBV	1940577	2460372	4.11%	2.137%

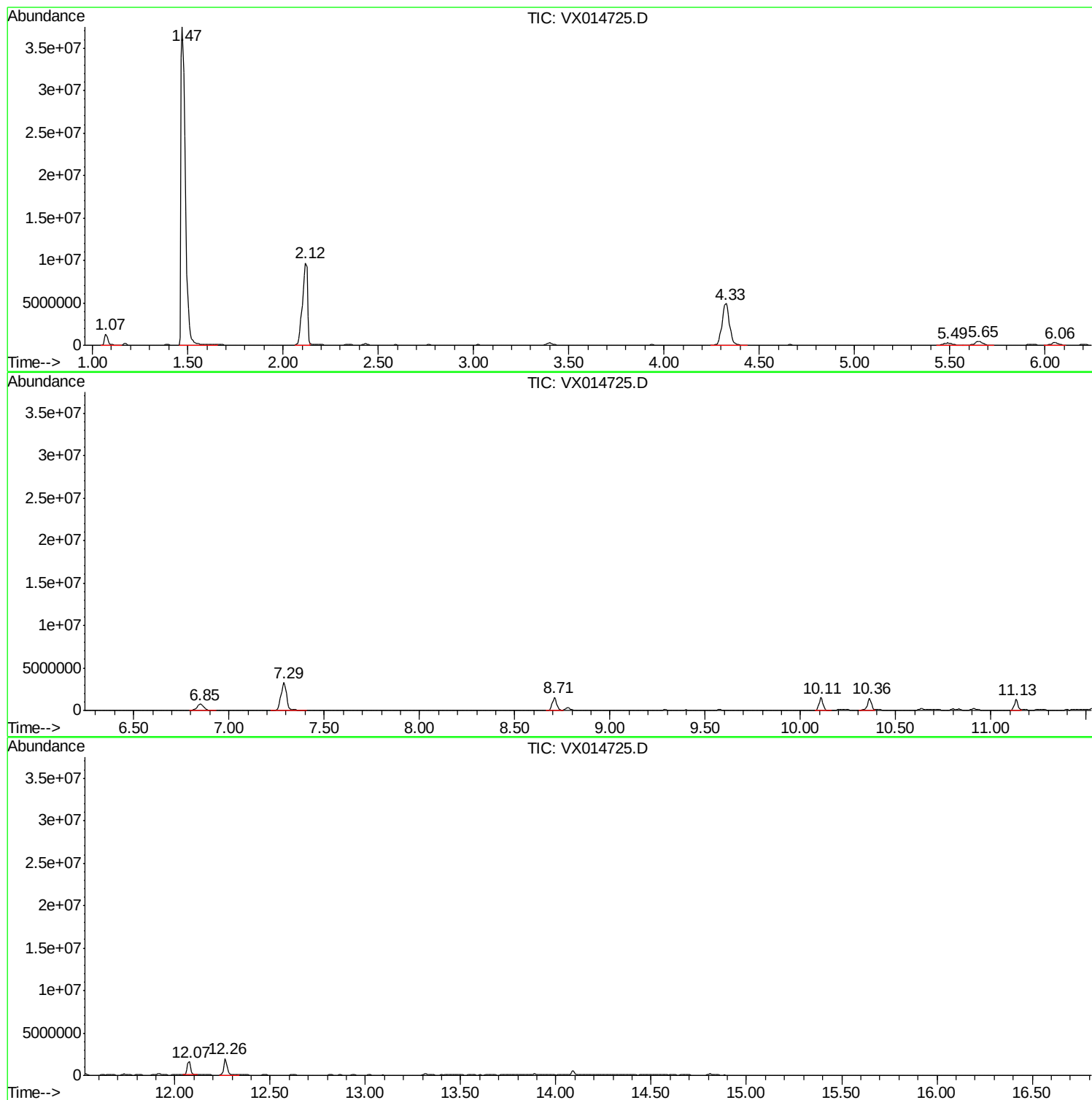
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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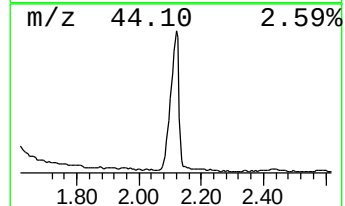
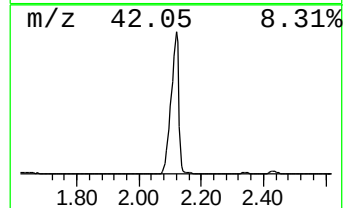
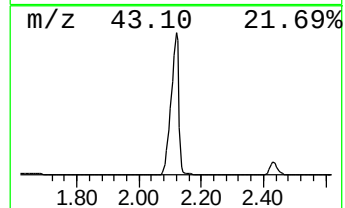
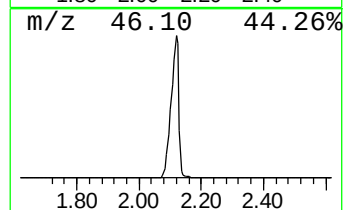
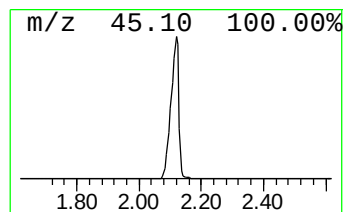
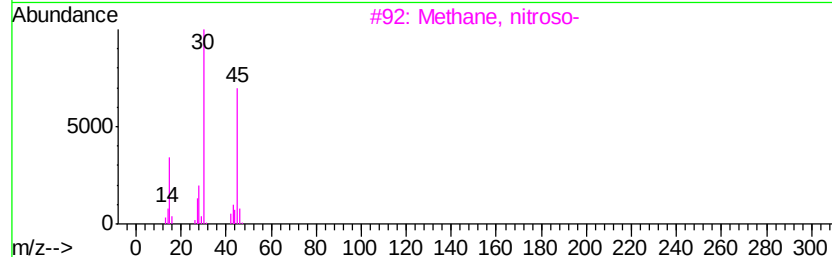
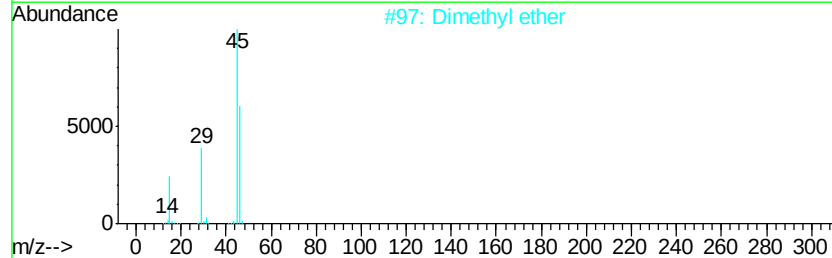
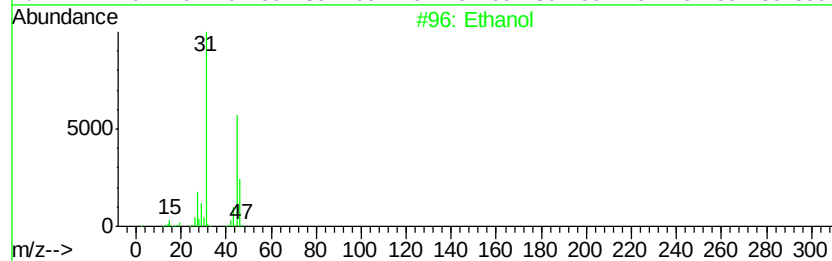
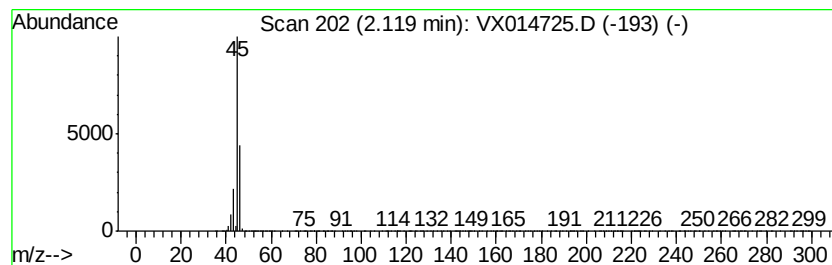
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X012220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	686.95 ug/l	17431400	Pentafluorobenzene	5.65

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol		46	C2H6O	000064-17-5	83
2	Dimethyl ether		46	C2H6O	000115-10-6	9
3	Methane, nitroso-		45	CH3NO	000865-40-7	4
4	Formic acid		46	CH2O2	000064-18-6	4
5	Oxalic acid		90	C2H2O4	000144-62-7	4



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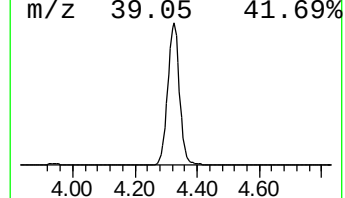
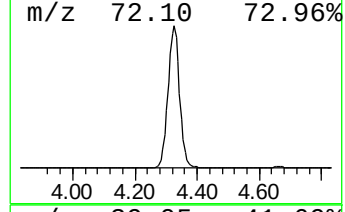
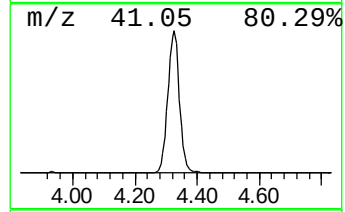
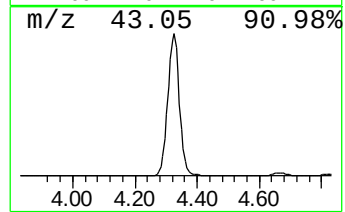
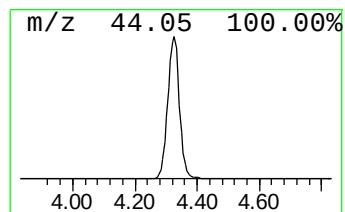
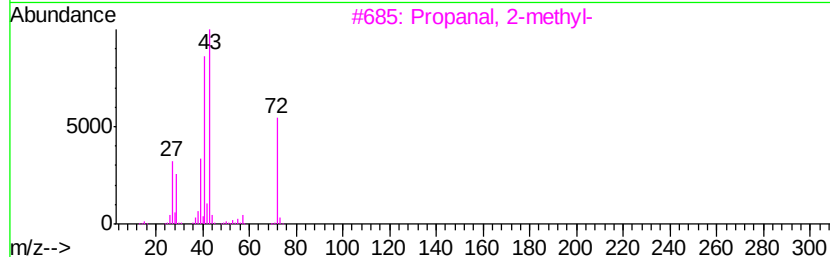
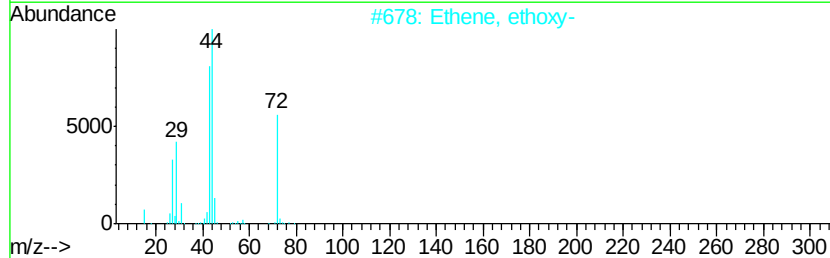
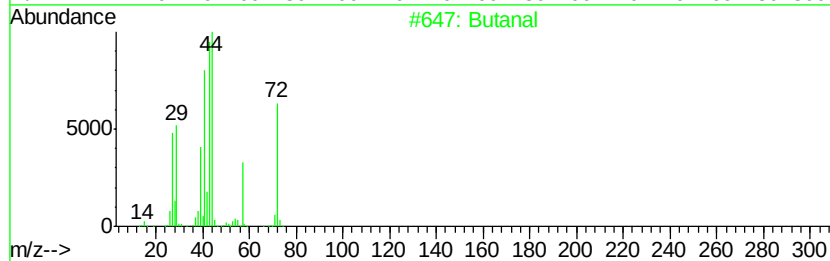
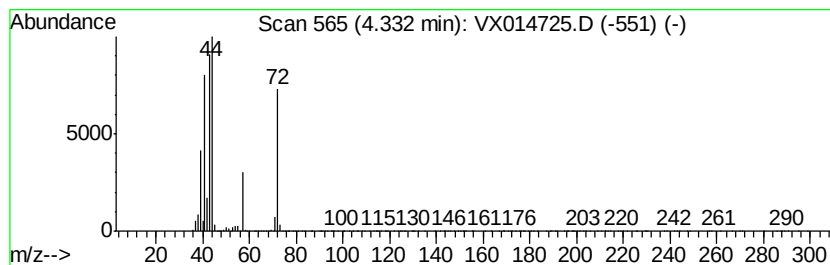
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Peak Number 4 Butanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.33	510.69 ug/l	12958800	Pentafluorobenzene	5.65

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal		72	C4H8O	000123-72-8	94
2	Ethene, ethoxy-		72	C4H8O	000109-92-2	52
3	Propanal, 2-methyl-		72	C4H8O	000078-84-2	50
4	1-Propene, 3-methoxy-		72	C4H8O	000627-40-7	32
5	Isobutylene epoxide		72	C4H8O	000558-30-5	22



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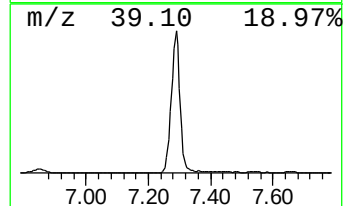
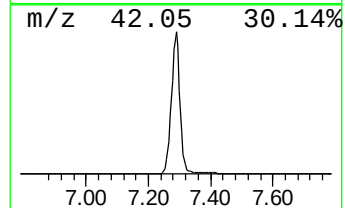
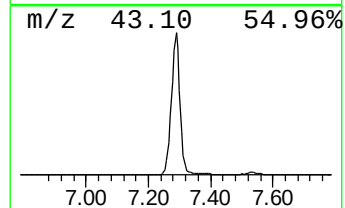
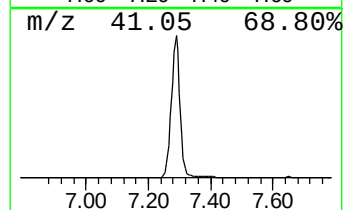
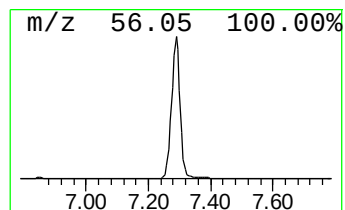
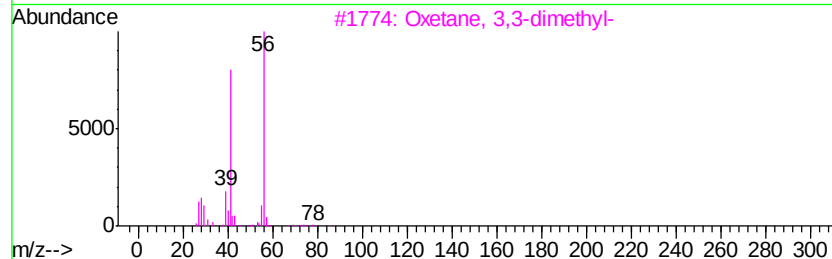
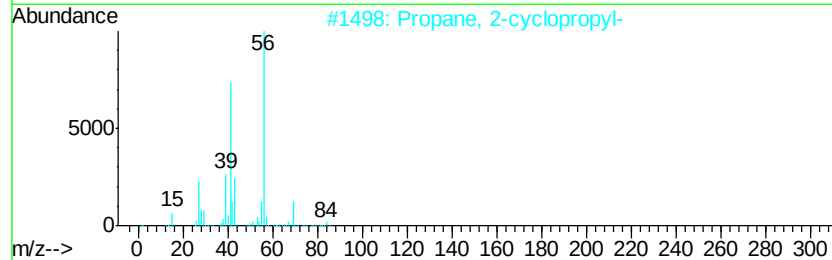
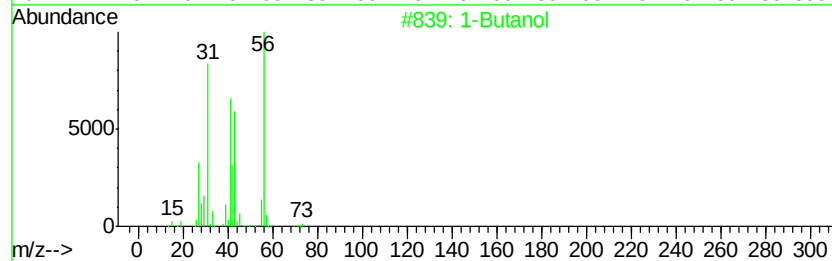
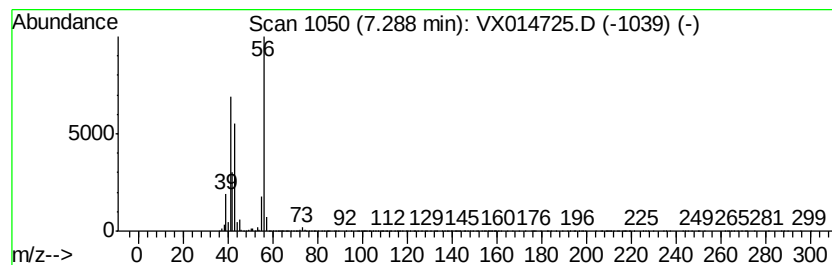
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Peak Number 5 1-Butanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.29	195.61 ug/l	6500610	1,4-Difluorobenzene	6.85

Hit# of	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	91
2	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	36
3	Oxetane, 3,3-dimethyl-	86	C5H10O	006921-35-3	9
4	Butane, 1-chloro-	92	C4H9Cl	000109-69-3	9
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	9



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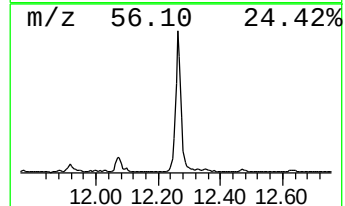
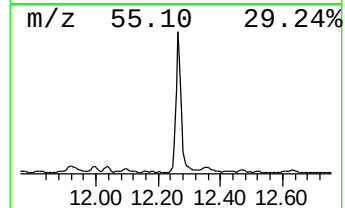
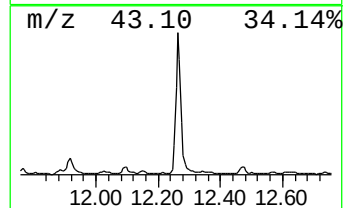
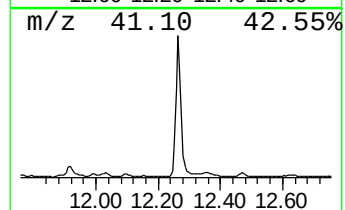
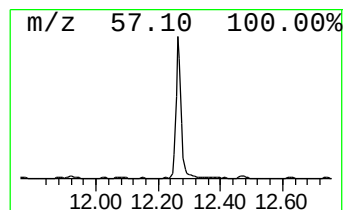
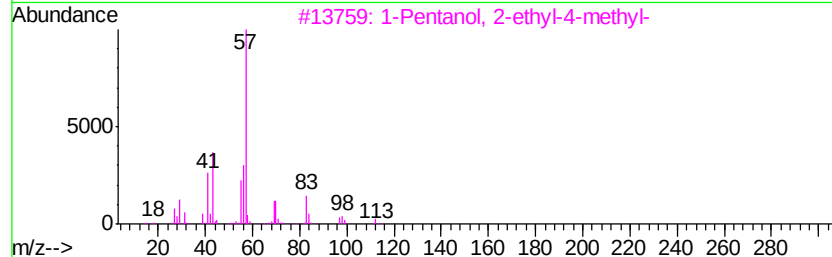
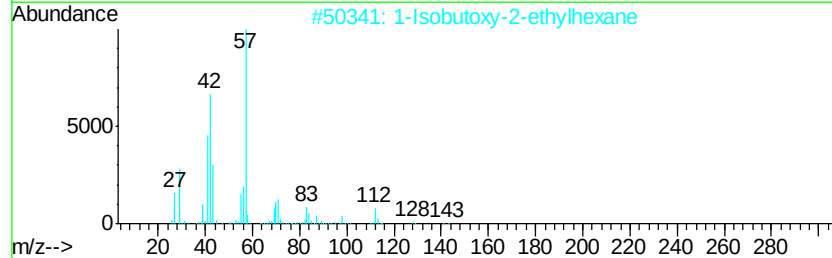
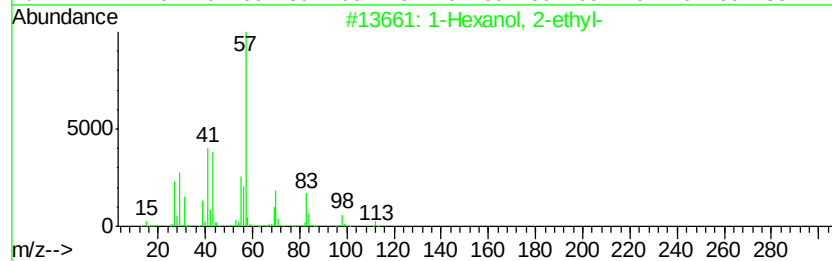
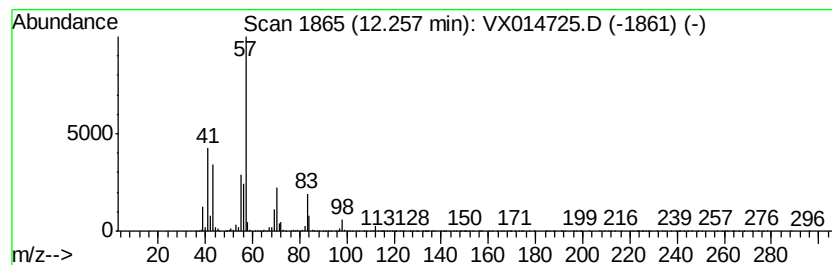
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Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	63.10 ug/l	2460370	1,4-Dichlorobenzene-d4	12.07

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2		1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
3		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
4		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
5		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50



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TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
Ethanol	2.12	687.0	ug/l	17431400	1	5.65	1268770	50.0
Butanal	4.33	510.7	ug/l	12958800	1	5.65	1268770	50.0
1-Butanol	7.29	195.6	ug/l	6500610	2	6.85	1661620	50.0
1-Hexanol, 2-ethyl-	12.26	63.1	ug/l	2460370	4	12.07	1949510	50.0